# TMVOC, A Simulator for Multiple Volatile Organic Chemicals

**Karsten Pruess and Alfredo Battistelli[1]**
[1]Aquater S.p.A., Italy
**Contact: Karsten Pruess, 510/486-6732, k_pruess@lbl.gov**

## RESEARCH OBJECTIVES

Many environmental contamination problems involve volatile organic chemicals (VOCs), such as crude oil, gasoline, diesel, and/or organic solvents. When spilled into the unsaturated zone, these chemicals may form a separate nonaqueous phase, giving rise to three-phase flow of water, soil gas, and a nonaqueous phase liquid (NAPL). Such flows can be modeled with T2VOC, but that code is limited to conditions in which the VOC is a pure, single-component fluid. However, in many cases of interest, nonaqueous fluids released into the subsurface may consist of a multicomponent mixture of several different chemicals. TMVOC is designed for three-phase flows in which the NAPL consists of a general multicomponent mixture of organic fluids. In addition, one or several noncondensable gases (NCGs) may be present.

## APPROACH

TMVOC is based on the M2NOTS code that was developed by Adenekan (1992) as part of his Ph.D. project at the University of California, Berkeley. It is implemented as a specialized module for Berkeley Lab's general multipurpose simulator TOUGH2 and retains its general process-modeling capabilities and user features.

## ACCOMPLISHMENTS

In the TMVOC formulation, the multiphase system is assumed to be composed of water, NCGs, and water-soluble VOCs. The number and nature of NCGs and VOCs can be specified by the user. Organic chemicals with critical temperatures below ambient, such as methane or ethane, can be modeled as NCGs. There are no intrinsic limitations to the number of NCGs or VOCs. Thermophysical property data for individual VOCs must be provided by the user. TMVOC uses a very general formulation to obtain thermophysical and PVT (pressure-volume-temperature) properties for mixtures of VOCs and NCGs. The fluid components may partition (volatilize and/or dissolve) among gas, aqueous, and NAPL phases. Any combination of the three phases may be present, and phases may appear and disappear in the course of a simulation.

Flows can be nonisothermal, and may involve advective, diffusive, phase-partitioning, and sorptive processes. A simple model for biodegradation is provided as well. Chief applications for which TMVOC is designed include analysis of NAPL spills and remediation alternatives in the vadose zone and below the water table.

A detailed self-contained user's guide is available that provides a technical reference to the TMVOC formulation and includes seven sample problems to illustrate code applications:

1. Demonstrating initialization of different phase conditions
2. One-dimensional Buckley-Leverett flow
3. Diffusion
4. Steam displacement of TCE
5. Steam displacement of a benzene-toluene mixture
6. Air displacement of NAPL
7. NAPL spill in the unsaturated zone

TMVOC is upwardly compatible with T2VOC; that is, T2VOC input files can be executed with TMVOC.

## SIGNIFICANCE OF FINDINGS

The TMVOC code is available through DOE's Energy Science and Technology Software Center (see http://www-esd.lbl.gov/TOUGH2/tmvoc.html).

## RELATED PUBLICATIONS

Adenekan, A.E., Numerical modeling of multiphase transport of multicomponent organic contaminants and heat in the subsurface. PhD thesis, University of California at Berkeley, 1992.

Pruess, K. and A. Battistelli. TMVOC, a numerical simulator for three-phase non-isothermal flows of multicomponent hydrocarbon mixtures in saturated-unsaturated heterogeneous media. Berkeley Lab Report LBNL-49375, 2002.

## ACKNOWLEDGMENTS

This work was supported, in part, by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. Partial support was also provided by a grant from Aquater S.p.A. (ENI Group) to Berkeley Lab in the frame of the REPIS project, sponsored by the ENI Research Fund.